Fixed-order predictions for top-quark pair production and decay at the LHC $\ensuremath{\mathsf{LHC}}$

Cavendish/DAMTP seminar

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NNLO QCD ingredients and technologies

- Introduction / Generalities (recap)
- STRIPPER IR subtraction framework (probably unfamiliar)

 \Downarrow Phenomenological application

Top-quark pair production and decay @ LHC

- Stable top-quark production (review)
- Production \otimes decay (pheno)
 - Leptonic differential distributions
 - Spin-correlation observables

Kinematical features

Experimental precision

WHY SHOULD WE CARE ABOUT NNLO QCD?

Perturbative

convergence

New channels

Fixed-order: Collider observables in QCD

- any process at colliders is specified by final states, and cuts on these final states
- parton-hadron duality is used, but partons being massless can be emitted at will
- it is necessary to sum (incoherently) over processes with a different number of final partons



• exchange or emission of partons lead to divergences



virtual - UV/IR

virtual momentum arbitrarily

large/small



real - IR soft

gluon energy arbitrarily small



real - IR collinear

angle between partons arbitrarily

small

Fixed-order: Kinoshita-Lee-Nauenberg theorem

- the theorem states that for "suitably averaged" transition probabilities (cross sections), the result is finite
- particular case is given by electron-positron annihilation



- after cuts: the different contributions are divergent, but the self energy itself is finite, and the total cross-section is just its imaginary part
- the averaging is obtained by integrating the cross section with a "jet function" F_n dependent on the momenta of the partons (or mesons and hadrons)
- F_n is required to be "infrared safe", i.e. the value for a soft or collinear degenerate configuration of n + 1 is the same as the value for the equivalent n partons

Fixed-order: Collinear factorization

- unfortunately, in hadronic collisions, the initial states are not properly averaged
- instead a factorization theorem is used, e.g. for top quark pair production:



$$\begin{split} \sigma_{h_1h_2 \to t\bar{t}}(s, m_t^2) &= \sum_{ij} \int_0^1 \int_0^1 dx_1 dx_2 \\ \phi_{i, h_1}(x_1, \mu_F^2) \phi_{j/h_2}(x_2, \mu_F^2) \hat{\sigma}_{ij}(\hat{s}, m_t^2, \alpha_s(\mu_R^2), \mu_R^2, \mu_F^2) \end{split}$$

- the divergences of the initial state collinear radiation are absorbed into the (universal) parton distribution functions
- the general formula is

$$\begin{bmatrix} \sigma_{ij}(x)/x \end{bmatrix} = \sum [\hat{\sigma}_{kl}(z)/z] \otimes \Gamma_{ki} \otimes \Gamma_{lj} \qquad \begin{bmatrix} f_1 \otimes f_2 \end{bmatrix} (x) = \int_0^1 dx_1 dx_2 f_1(x_1) f_2(x_2) \delta(x - x_1 x_2) \\ \Gamma_{ij} = \delta_{ij} \delta(1 - x) - \frac{\alpha_s}{\pi} \frac{P_{ij}^{(0)}(x)}{\epsilon} + \left(\frac{\alpha_s}{\pi}\right)^2 \left[\frac{1}{2\epsilon^2} \left(\left(P_{ik}^{(0)} \otimes P_{kj}^{(0)} \right) (x) + \beta_0 P_{ij}^{(0)}(x) \right) - \frac{1}{2\epsilon} P_{ij}^{(1)}(x) \right] + \mathcal{O}\left(\alpha_s^3\right)$$

• Consistency of the construction requires a consistent dimensional regularization

• add to the original cross section $\sigma = \sigma^{LO} + \sigma^{NLO}$

$$\sigma^{LO} = \int_m \mathrm{d}\sigma^B \quad , \qquad \sigma^{NLO} \equiv \int \mathrm{d}\sigma^{NLO} = \int_{m+1} \mathrm{d}\sigma^R + \int_m \mathrm{d}\sigma^V$$

an identity involving approximations to the real radiation cross section

$$\sigma^{\textit{NLO}} = \int_{m+1} \left[\mathrm{d}\sigma^{R} - \mathrm{d}\sigma^{A} \right] + \int_{m+1} \mathrm{d}\sigma^{A} + \int_{m} \mathrm{d}\sigma^{V}$$

and regroup the terms as

$$\sigma^{NLO} = \int_{m+1} \left[\left(\mathrm{d}\sigma^R \right)_{\epsilon=0} - \left(\mathrm{d}\sigma^A \right)_{\epsilon=0} \right] + \int_m \left[\mathrm{d}\sigma^V + \int_1 \mathrm{d}\sigma^A \right]_{\epsilon=0}$$

- for $d\sigma^A$ it must be possible to
 - obtain the Laurent expansion by integration over the single particle unresolved space (preferably analytically)
 - 2. approximate $d\sigma^R$ (preferably pointwise)

NLO Subtraction Schemes

- Dipole Subt. [Catani,Seymour'98]
- FKS [Frixione,Kunst,Signer'95]
- Antenna Subtraction [Kosower'97]
- Nagy-Soper [Nagy,Soper'07]

Generalization to NNLO?

- Nature of singularities known: soft and collinear limits
- NLO (fairly simple):
 - single soft
 - single collinear
- At NNLO? : Many (overlapping) ways to reach soft and collinear limits
- Possible way: Decomposition of the phase space to disentangle them

Handling real radiation contribution in NNLO calculations cancellation of infrared divergences

increasing number of available NNLO calculations with a variety of schemes

• qT-slicing [Catani, Grazzini, '07], [Ferrera, Grazzini, Tramontano, '11], [Catani, Cieri, DeFlorian, Ferrera, Grazzini, '12],

[Gehrmann, Grazzini, Kallweit, Maierhofer, Manteuffel, Rathlev, Torre, '14-15'], [Bonciani, Catani, Grazzini, Sargsyan, Torre, '14-'15]

- N-jettiness slicing [Gaunt,Stahlhofen,Tackmann,Walsh, '15], [Boughezal,Focke,Giele,Liu,Petriello,'15-'16], [Bougezal,Campell,Ellis,Focke,Giele,Liu,Petriello,'15], [Campell,Ellis,Williams,'16]
- Antenna subtraction [Gehrmann, GehrmannDeRidder, Glover, Heinrich, '05-'08], [Weinzierl, '08, '09],

[Currie,Gehrmann,GehrmannDeRidder,Glover,Pires,'13-'17], [Bernreuther,Bogner,Dekkers,'11,'14],

[Abelof, (Dekkers), GehrmannDeRidder, '11-'15], [Abelof, GehrmannDeRidder, Maierhofer, Pozzorini, '14],

[Chen, Gehrmann, Glover, Jaquier, '15]

- Colorful subtraction [DelDuca,Somogyi,Troscanyi,'05-'13], [DelDuca,Duhr,Somogyi,Tramontano,Troscanyi,'15]
- Sector-improved residue subtraction (STRIPPER) [Czakon, '10, '11] .

[Czakon,Fiedler,Mitov,'13,'15], [Czakon,Heymes,'14] [Czakon,Fiedler,Heymes,Mitov,'16,'17],

[Bughezal, Caola, Melnikov, Petriello, Schulze, '13, '14], [Bughezal, Melnikov, Petriello, '11],

[Caola, Czernecki, Liang, Melnikov, Szafron, '14], [Bruchseifer, Caola, Melnikov, '13-'14], [Caola, Melnikov, Röntsch, '17]

• . . .

Sector-improved residue subtraction

Hadronic cross section:

 $\sigma_{h_1h_2}(P_1, P_2) = \sum \iint_0^1 \mathrm{d}x_1 \,\mathrm{d}x_2 \,f_{a/h_1}(x_1, \mu_F^2) f_{b/h_2}(x_2, \mu_F^2) \hat{\sigma}_{ab}(x_1P_1, x_2P_2; \alpha_S(\mu_R^2), \mu_R^2, \mu_F^2)$

partonic cross section:

$$\hat{\sigma}_{ab} = \hat{\sigma}_{ab}^{(0)} + \hat{\sigma}_{ab}^{(1)} + \hat{\sigma}_{ab}^{(2)} + \mathcal{O}\left(\alpha_{S}^{3}\right)$$

Contributions with different final state multiplicities and convolutions:

$$\hat{\sigma}_{ab}^{(2)} = \hat{\sigma}_{ab}^{\text{RR}} + \hat{\sigma}_{ab}^{\text{RV}} + \hat{\sigma}_{ab}^{\text{VV}} + \hat{\sigma}_{ab}^{\text{C2}} + \hat{\sigma}_{ab}^{\text{C1}}$$

$$\begin{split} \hat{\sigma}_{ab}^{\mathrm{RP}} &= \frac{1}{2\hat{s}} \int \mathrm{d}\Phi_{n+2} \left\langle \mathcal{M}_{n+2}^{(0)} \middle| \mathcal{M}_{n+2}^{(0)} \right\rangle \mathbf{F}_{n+2} & \hat{\sigma}_{ab}^{\mathrm{C1}} = (\text{single convolution}) \mathbf{F}_{n+1} \\ \hat{\sigma}_{ab}^{\mathrm{RV}} &= \frac{1}{2\hat{s}} \int \mathrm{d}\Phi_{n+1} \operatorname{2Re} \left\langle \mathcal{M}_{n+1}^{(0)} \middle| \mathcal{M}_{n+1}^{(1)} \right\rangle \mathbf{F}_{n+1} & \hat{\sigma}_{ab}^{\mathrm{C2}} = (\text{double convolution}) \mathbf{F}_{n} \\ \hat{\sigma}_{ab}^{\mathrm{VV}} &= \frac{1}{2\hat{s}} \int \mathrm{d}\Phi_{n} \left(\operatorname{2Re} \left\langle \mathcal{M}_{n}^{(0)} \middle| \mathcal{M}_{n}^{(2)} \right\rangle + \left\langle \mathcal{M}_{n}^{(1)} \middle| \mathcal{M}_{n}^{(1)} \right\rangle \right) \mathbf{F}_{n} \end{split}$$

Several layers of decomposition

Selector functions:

$$1 = \sum_{i,j} \left[\sum_{k} \mathcal{S}_{ij,k} + \sum_{k,l} \mathcal{S}_{i,k;j,l} \right]$$

Factorization of double soft limits:

$$\theta(u_1^0 - u_2^0) + \theta(u_2^0 - u_1^0)$$

Sector parameterization Parameterization with respect to the reference parton *r*: angles: $\hat{\eta}_i = \frac{1}{2}(1 - \cos \theta_{ir}) \in [0, 1]$ energies: $\hat{\xi}_i = \frac{u_i^0}{u_{max}^0} \in [0, 1]$



STRIPPER: Compilation

$$\begin{split} \hat{\sigma}_{ab}^{\text{RP}} &= \frac{1}{2\hat{s}} \int d\Phi_{n+2} \left\langle \mathcal{M}_{n+2}^{(0)} \middle| \mathcal{M}_{n+2}^{(0)} \right\rangle F_{n+2} \\ \hat{\sigma}_{ab}^{\text{RV}} &= \frac{1}{2\hat{s}} \int d\Phi_{n+1} 2\text{Re} \left\langle \mathcal{M}_{n+1}^{(0)} \middle| \mathcal{M}_{n+1}^{(1)} \right\rangle F_{n+1} \\ \hat{\sigma}_{ab}^{\text{CU}} &= \frac{1}{2\hat{s}} \int d\Phi_n \left(2\text{Re} \left\langle \mathcal{M}_n^{(0)} \middle| \mathcal{M}_n^{(2)} \right\rangle + \left\langle \mathcal{M}_n^{(1)} \middle| \mathcal{M}_n^{(1)} \right\rangle \right) F_n \end{split}$$

Sector decomposition and master formula:

$$x^{-1-b\epsilon} = \underbrace{\frac{-1}{b\epsilon}}_{\text{pole term}} + \underbrace{\left[x^{-1-b\epsilon}\right]_{+}}_{\text{reg. + sub.}}$$

₽

$$\begin{pmatrix} \sigma_{F}^{RR}, \sigma_{SU}^{RR}, \sigma_{DU}^{RV} \end{pmatrix} \quad \begin{pmatrix} \sigma_{F}^{RV}, \sigma_{SU}^{RV}, \sigma_{DU}^{RV} \end{pmatrix} \quad \begin{pmatrix} \sigma_{F}^{VV}, \sigma_{DU}^{VV}, \sigma_{FR}^{VV} \end{pmatrix} \quad \begin{pmatrix} \sigma_{SU}^{C1}, \sigma_{DU}^{C1} \end{pmatrix} \quad \begin{pmatrix} \sigma_{C1}^{C2}, \sigma_{C2}^{C2} \end{pmatrix}$$

 \Downarrow 4 dimensional formulation [Czakon, Heymes'14]

$$\begin{pmatrix} \sigma_{F}^{RR} \end{pmatrix} \quad \begin{pmatrix} \sigma_{F}^{VV} \end{pmatrix} \quad \begin{pmatrix} \sigma_{F}^{RV} \end{pmatrix} \quad \begin{pmatrix} \sigma_{SU}^{RR}, \sigma_{SU}^{RV}, \sigma_{SU}^{C1} \end{pmatrix} \quad \begin{pmatrix} \sigma_{DU}^{RR}, \sigma_{DU}^{RV}, \sigma_{DU}^{VV}, \sigma_{DU}^{C1}, \sigma_{DU}^{C2} \end{pmatrix} \quad \begin{pmatrix} \sigma_{FR}^{RV}, \sigma_{FR}^{VV}, \sigma_{FR}^{C2} \end{pmatrix} \quad \begin{pmatrix} \sigma_{FR}^{RV}, \sigma_{FR}^{VV}, \sigma_{FR}^{VV}, \sigma_{FR}^{VV} \end{pmatrix} \quad \begin{pmatrix} \sigma_{FR}^{RV}, \sigma_{FR}^{VV}, \sigma_{FR}^{VV}, \sigma_{FR}^{VV}, \sigma_{FR}^{VV}, \sigma_{FR}^{VV} \end{pmatrix} \quad \begin{pmatrix} \sigma_{FR}^{RV}, \sigma_{FR}^{VV}, \sigma_{FR}^{VV}, \sigma_{FR}^{VV}, \sigma_{FR}^{VV}, \sigma_{FR}^{VV}, \sigma_{FR}^{VV}, \sigma_{FR}^{VV}, \sigma_{FR}^{VV}, \sigma_{FR}^{VV} \end{pmatrix}$$

• new phase space parameterization:

- reduced mis-binning
- new 4-dimensional formulation
- *ϵ*-pole cancelation PS point wise (strong check of construction/implementation)

• C++ framework:

- automatic generation of necessary contributions/subtraction-terms
- only one- and two-loop amplitutes as external input (OpenLoops/Recola interfaces)
- flexible 'measurement'-system (fastNLO tables, smearing techniques, efficient scale and PDF variation)

Top quark pair production and decay

Top-quark production at the LHC

- Heaviest known particle \rightarrow special place in the SM
- Abundantly produced at the LHC
 - \rightarrow top-quark factory
 - \rightarrow high quality and precision data
- Many opportunities to study QCD/SM in high precision
- Many connections to other fields: Higgs, BSM, EW precision



State-of-the-art: Total cross section for $t\bar{t}$ production

- NNLO QCD + NNLL soft gluon resummation
- Uncertainties of a few percent
- Remarkable agreement with measurements at 7, 8 and 13 TeV



State-of-the-art: Differential $t\bar{t}$ cross sections @ NNLO QCD





NNLO QCD

- Modification of shape for p_T and m_{tt}
- Reduction of scale dependence
- choice of dynamical scale is crucial
 - \rightarrow extensive study of perturbative convergence





arxiv:1606.03350 [Czakon,Heymes,Mitov '16]

- Renormalization/Factorization scale dependence \rightarrow major source of theory uncertainty
- What is a sensible scale choice? → possible metric: principle of fasted convergence
- Total cross section: $\mu = m_t/2$
- Differential cross sections? Probing a vast energy regime ⇒ dynamical scales
- *H*_T/4 established for most observables (except *m*_T/2 for *p*_{T,t} distributions)

arxiv:1606.03350 [Czakon,Heymes,Mitov '16]



State-of-the-art: Resummation for differential observables

- Advances in resummation for differential observables
- Threshold (low p_T) and small-mass (high p_T 'boosted tops') logarithms
- Stabilizes results w.r.t. scale choice form
- Results support $H_T/4$ as the 'best' scale since $H_T/4$ seems to capture most of the resummation features





arxiv:1803.07623 [Czakon, Ferroglia, Heymes, Mitov, Pecjak, Scott, Wang, Yang '18]

State-of-the-art: NLO-EW corrections

- Studied in additive and multiplicative approach
- Observed strong PDF dependence
- Size of corrections are observable dependent: $p_{T,avt}$: up to -25% at high p_T (Sudakov logarithms),

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> NNLO QCD scale dependence for p_{T, \textit{avt}} > 500 GeV
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y_t, y_{t\bar{t}}: small effect (< NNLO QCD scale dependence)
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 multiplicative approach results in smaller scale dependence

arxiv:1705.04105 [Czakon, Heymes, Mitov, Pagani, Tsinikos, Zaro '17]



Production and decay

Elephant in the room:

Top-quarks are not stable and are measured utilising the decay products

- Decay products are measured in fiducial phase space \to all previous results rely on the extrapolation of the phase space
- The phase space extrapolation relies heavily on MC modeling of the top-quark production and its decay
- The modeling might have more or less subtle impacts on results derived in the extrapolated phase space

Narrow-Width-Approximation

- Considering limit $\Gamma_t \to 0$
- Factorization of production and decay
- Reduction of complexity by keeping crucial features of decay like spin-correlations
- Expected error of $\mathcal{O}(\Gamma_t/m_t)$

Off-shell calculations

- Considering the complete process: $pp \rightarrow \ell^+ \ell^- \nu \bar{\nu} b \bar{b} + X$
- Technically challenging due to high multiplicity, difficult phase space
- Off-shell and non-resonant effects important in certain phase space region



Production and decay: NLO for off-shell $t\bar{t}$

- NLO corrections to full $pp \rightarrow \ell^+ \ell^- \nu \bar{\nu} b \bar{b} + X$ [5FS: Bevilacqua et al, Denner et al, Heinrich et al, 4FS: Frederix, Cascioli et al]
- Off-shell & non-resonant effects depend strongly on observable
- $\bullet \ \rightarrow \ \mathsf{NWA} \ \mathsf{approximation} \ \mathsf{valid} \ \mathsf{for} \\ \mathsf{many} \ \mathsf{observables}$
- Higher order corrections to decay are important!
- Kinematical thresholds and edges are sensitive to off-shell effects ⇒ NWA does not give a valid description



Production and decay: NLO + PS for off-shell $t\bar{t}$





- $\bullet\,$ Matching fixed order calculation to PS
- Technical subtlety: resonance-aware matching. Implementation in POWHEG framework
- Detailed comparison of:
 - "*tt*": NWA, NLO production only (industry standard)
 - " $t\bar{t}\otimes$ decay": NWA, NLO production & decay , approximate LO finite width effects

[Campbell,Ellis,Nason,Re '14]

*"bb*4ℓ": full off-shell

[Jezo, Nason '15] [Jezo, Lindert, Nason, Oleari, Pozzorini '16]

- Upshot:
 - " $t\bar{t} \otimes$ decay" closer to " $b\bar{b}4\ell$ " than " $t\bar{t}$ " (in terms of shape and normalization)
 - NLO corrections to decay are crucial for NWA to be reliable to work

Production and decay: Narrow-Width-Approximation

• top-quark have a short life time, decay before hadronization. $\Gamma_t \ll m_t$

$$\frac{1}{(p^2-m_t^2)^2+m_t^2\Gamma_t^2} \xrightarrow{\Gamma_t/m_t\to 0} \frac{\pi\delta(p^2-m_t^2)}{m_t\Gamma_t}$$

• for on-shell top-quarks:

$$\not p + m_t = \sum_{\lambda} u_{\lambda}(p) \bar{u}_{\lambda}(p)$$

- factorization of production and decay
- polarized matrix elements required





- NNLO QCD correction to NWA with leptonic decays now available
- Extension of the STRIPPER framework used for differential $t\bar{t}$
- Predictions for inclusive and fiducial phase spaces
- Many applications in work: leptonic distributions, top-quark (differential) cross sections in fiducial phase space, top-quark mass extraction
- Study of top-quark spin-correlation

- comparision between CMS data [CMS,1505.04480] and NWA @ NNLO QCD
- good discribtion of many distributions:
 - transverse momentum of ℓ and b-jets



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 - rapidities of ℓ and b-jets



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 - $\bullet~$ rapidities of $\ell~$ and b-jets
 - transverse momentum of lepton and b-jet pairs



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- good discribtion of many distributions:
 - transverse momentum of ℓ and b-jets
 - $\bullet~$ rapidities of $\ell~$ and b-jets
 - transverse momentum of lepton and b-jet pairs
 - invariant masses of lepton and b-jet pairs



Production and decay: Spin-correlation @ NNLO QCD

- Direct measurement of top-quark spin density matrix [CMS,PAS TOP-18-006]
 - full spin information
 - systematic difficulties (neutrinos → top-momenta)
- Leptonic observables are sensitive to $t\bar{t}$ spin-correlations. For example the opening angles of the leptons: $\Delta \Phi_{\ell\ell}$ and $|\Delta \eta_{\ell\ell}|$
- Boosted top favor antiparallel leptons
- Spin correlation counter acts
- Effect of higher corrections?





Production and decay: Spin-correlation @ NNLO QCD

Fiducial phase space

LHC 13 TeV m_l = 172.5 GeV Scale: Hg/4 PDF: NNPDF31mlo Scale: H_T/4 PDF: NNPDF31mlc --- LO - NNLO --- LO - NNLO - NLO ATLAS - NLO ATLAS inclusive fiducial 3 $|\Delta \eta(\ell, \tilde{\ell})|$ $|\Delta \eta(\ell, \bar{\ell})|$ $d(\Delta \phi/\pi)$ -- LO NNLO Fiducial $dr / d(\Delta \phi/\pi)$ LO - NNLO Inclusive NLO . ATLAS NLO ATLAS LHC 13 TeV $m_t = 172.5$ GeV LHC 13 TeV $m_l = 172.5$ GeV Scale: $H_T/4$ PDF: NNPDF31nulo Scale: Hy/4 PDF: NNPDF31nnle 01N/0 OIN/OINN R 0.92 NLO/LO ٠ $\Delta \phi(\ell, \bar{\ell})/\pi$ $\Delta \phi(\ell, \bar{\ell})/\pi$

Inclusive phase space

arxiv:1901.05407 [Behring,Czakon,Mitov,Papanastasiou,P '19]

Extrapolation effects?

Production and decay: Spin-correlation @ NNLO QCD

- $\bullet \ \rightarrow \ \text{extrapolation effect?}$
- Published results: [arXiv:1903.07570
 ATLAS '19] (discrepancy resolved by EW effects?)





arxiv:1901.05407 [Behring,Czakon,Mitov,Papanastasiou,P '19]

Summary & Outlook

Summary

- Top-quark production at the LHC is theoretically very well understood and under control and allows for precision test and parameter extraction of the SM
- Refined calculation (through resummation and/or NLO EW) allow to improve theoretical stability and understanding
- Precision calculations for more realistic final states including the top-quarks decay.
- NNLO QCD predictions including leptonic top-quark decays. Production cross sections and differential distributions in fiducial volumes.

Outlook

- Using precision predictions to get out as much as possible of LHC data
- SM model precision test and parameter estimations: m_t , α_s , PDFs,...
- Incoming NNLO QCD predictions including leptonic decays: differential distributions of decay products → overcome penalties of extrapolation